Dichloroacetylene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 37.5 °C

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

Image not found
Dichloroacetylene
Measured: 33.0
Predicted: 37.5

Image not found
Propargyl bromide
Measured: 89.0
Predicted: 74.4

Image not found
1-Propyne, 3-chloro-
Measured: 58.0
Predicted: 49.6

Image not found
Ethyne, chloro-
Measured: -30.0
Predicted: -21.3